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Nuclear Fission in Monte Carlo Particle Transport Simulations

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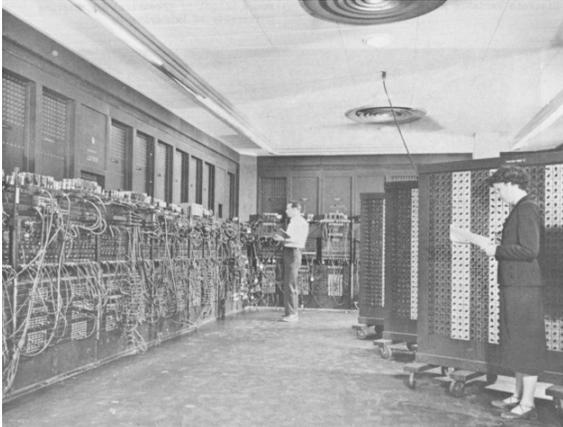
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Monte Carlo computer codes have been used to simulate neutron transport in fissionable materials since the late 1940s. Today's MC codes such as MCNP6 can accurately model nearly any geometry and make use of detailed physics interaction data from the ENDF/B- VII libraries. For many applications today, many billions of neutrons are simulated using MC methods on parallel computers. While MC methods for neutron transport can be viewed in practical terms (i.e., just simulate particle behavior), there is a solid mathematical and physical basis founded in the linear Boltzmann transport equation. This lecture provides an overview of MC methods for simulating particle transport, with particular emphasis on the fundamental assumptions in the underlying equations and transport and collision modeling. Depending on the application, some portions of the simulations may use expected-value outcomes, while other portions require detailed modeling that conserves energy, momentum, particles, correlations, etc. Static eigenvalue calculations are compared with fixed-source time dependent approaches, and the detailed modeling of fission processes in MCNP is reviewed.

- **Introduction**
- **Monte Carlo simulation and the transport equation**
 - Overview, particle simulation, theory, assumptions
 - Eigenvalue problems vs. fixed-source time dependent problems
- **Using expected-value outcomes vs. detailed modeling**
 - Analog vs weighted simulation
 - Transport process and Doppler broadening
 - Collision physics and particle production
- **Fission process modeling in MCNP**
 - Expected-value approach for eigenvalue calculations
 - Detailed modeling of multiplicity and correlated particle production
 - Spontaneous vs. induced fission
 - Emission spectra

Introduction

Monte Carlo & MCNP History

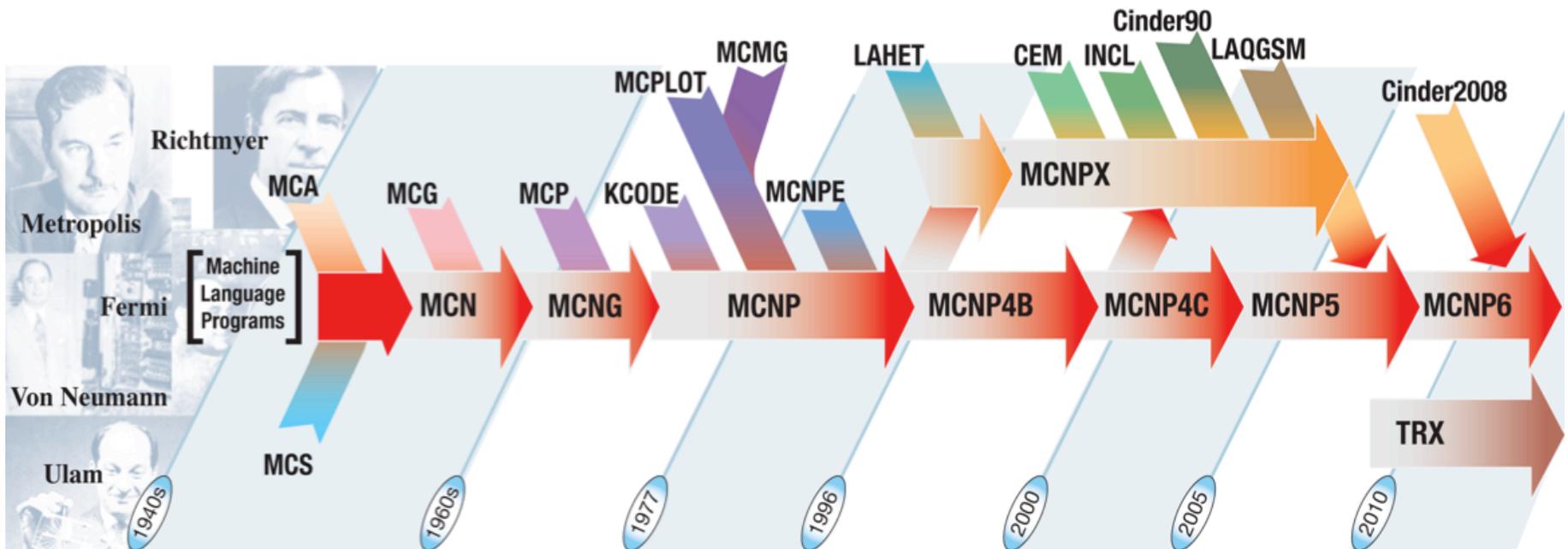


ENIAC – 1945

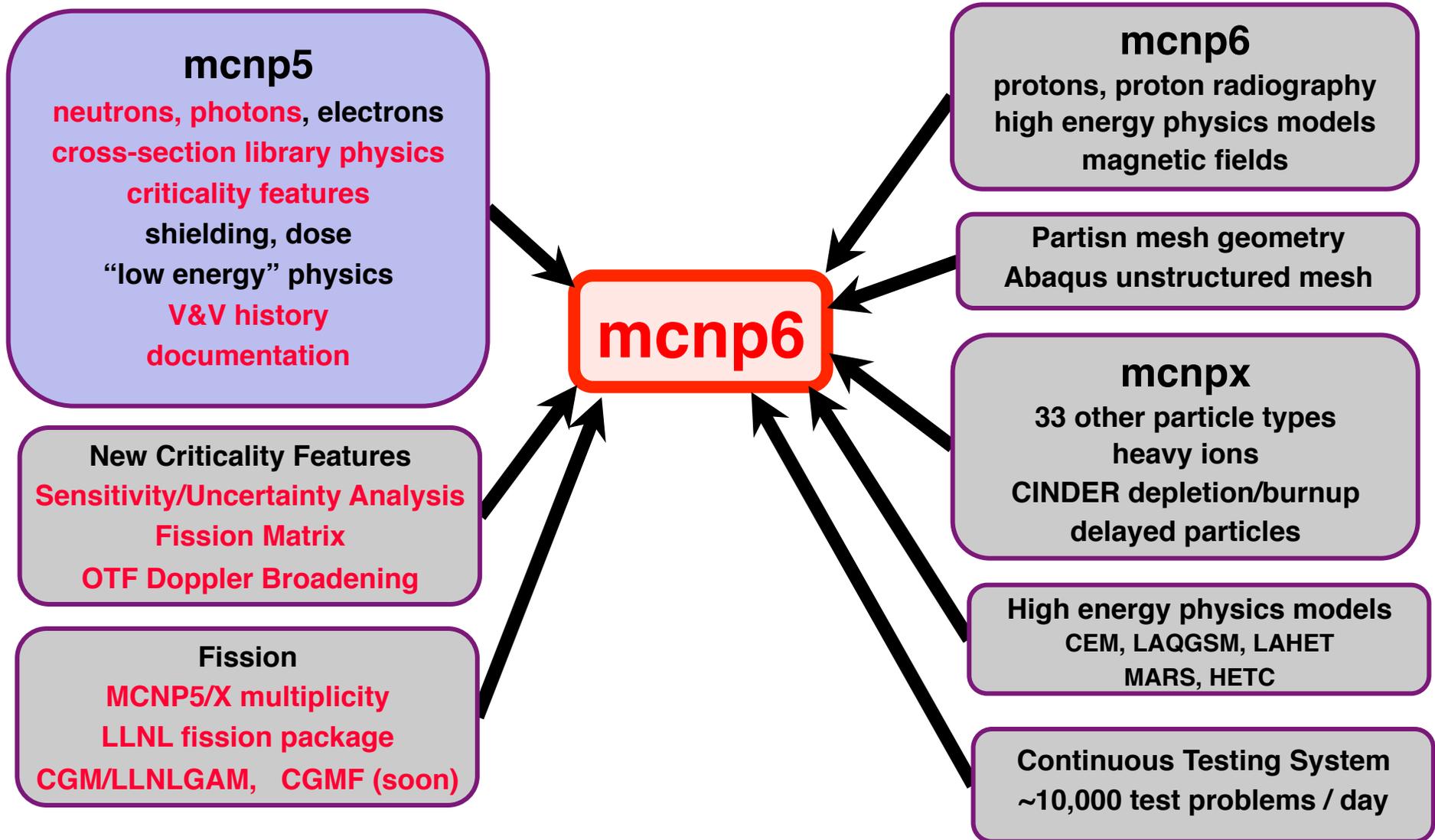
- 30 tons
- 20 ft x 40 ft room
- 18,000 vacuum tubes
- 0.1 MHz
- 20 word memory
- patchcords

Manhattan Project – 1945...

- Discussions on using ENIAC
- Ulam** suggested using the “method of statistical trials”
- Metropolis** suggested the name “Monte Carlo”
- Von Neumann** developed the first computer code



MCNP6 Features



mcnp5 – 100 K lines of code
mcnp6 – 500 K lines of code

MCNP & Nuclear Criticality Safety (1)

HEU-MET-THERM-003

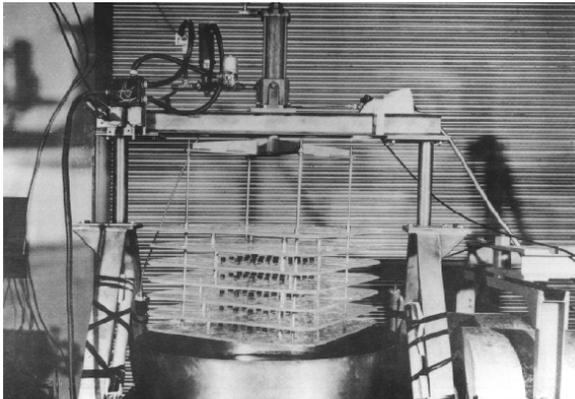
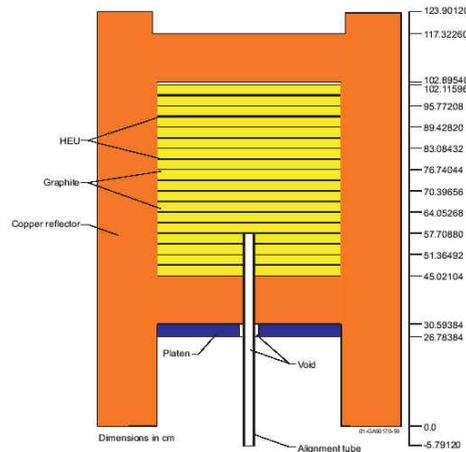
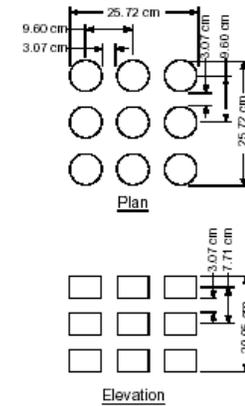


Figure 2. Array of 0.5-in. Cubes Prior to Immersion.

Zeus-2, HEU-MET-INTER-006, case 2



PU-MET-FAST-003, case 3



IEU-COMP-THERM-002, case 3

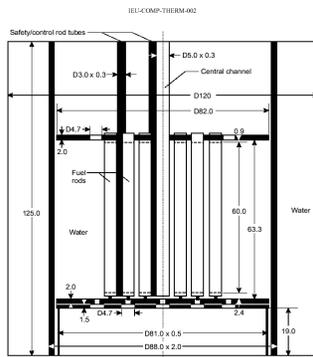
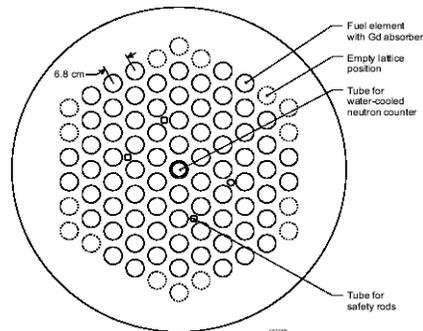


Figure 5. Model of Core.

(dimensions in cm; outer diameters are shown; the value "n" in the notation "n" is the wall thickness)

IEU-COMP-THERM-002



PNL-33 - MIX-COMP-THERM-002

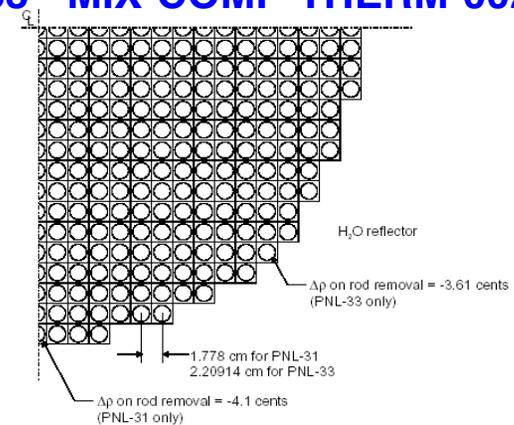


Figure 7. Fuel Loading for PNL-31 and PNL-33.

MCNP & Nuclear Criticality Safety (2)

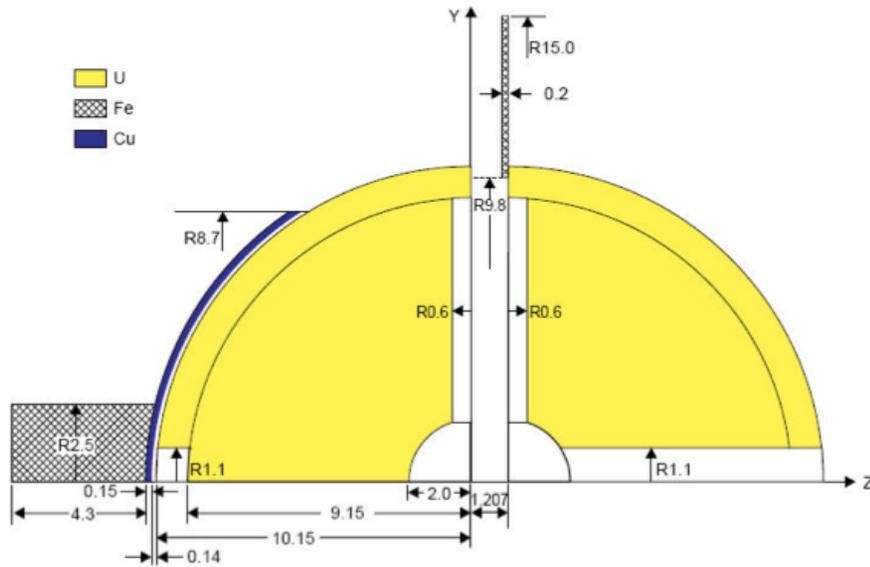


Figure 1. Unreflected HEU Sphere, heu-met-fast-008

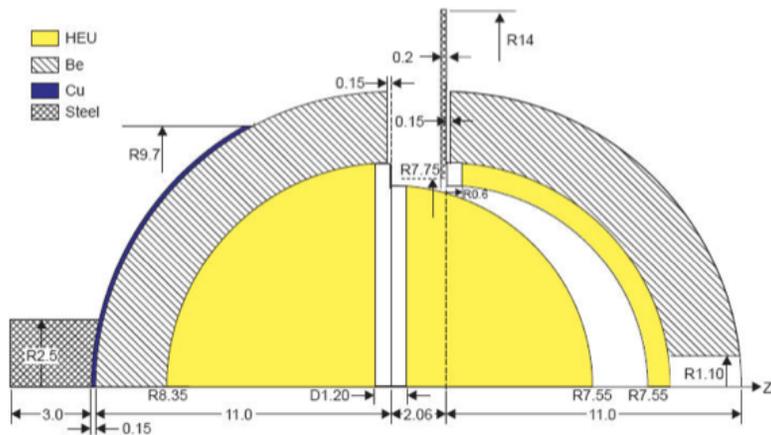


Figure 2. Incomplete HEU Sphere Reflected by Beryllium, heu-met-fast-009-case-1

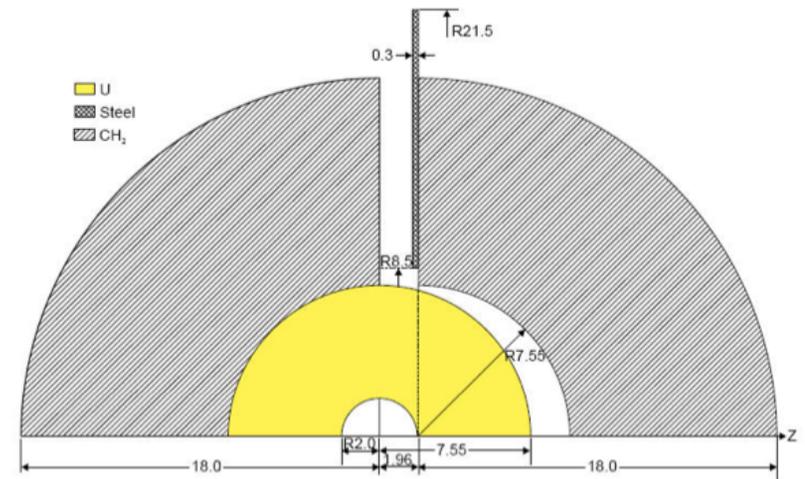


Figure 4. HEU Sphere Reflected by Polyethylene, heu-met-fast-011

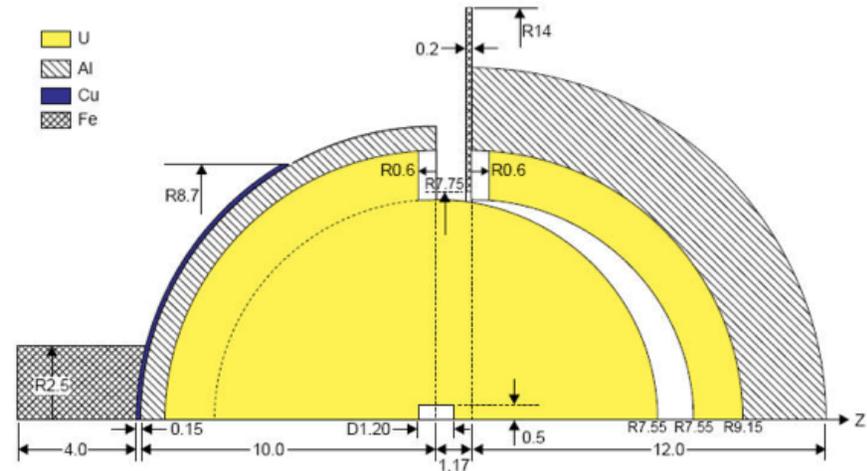
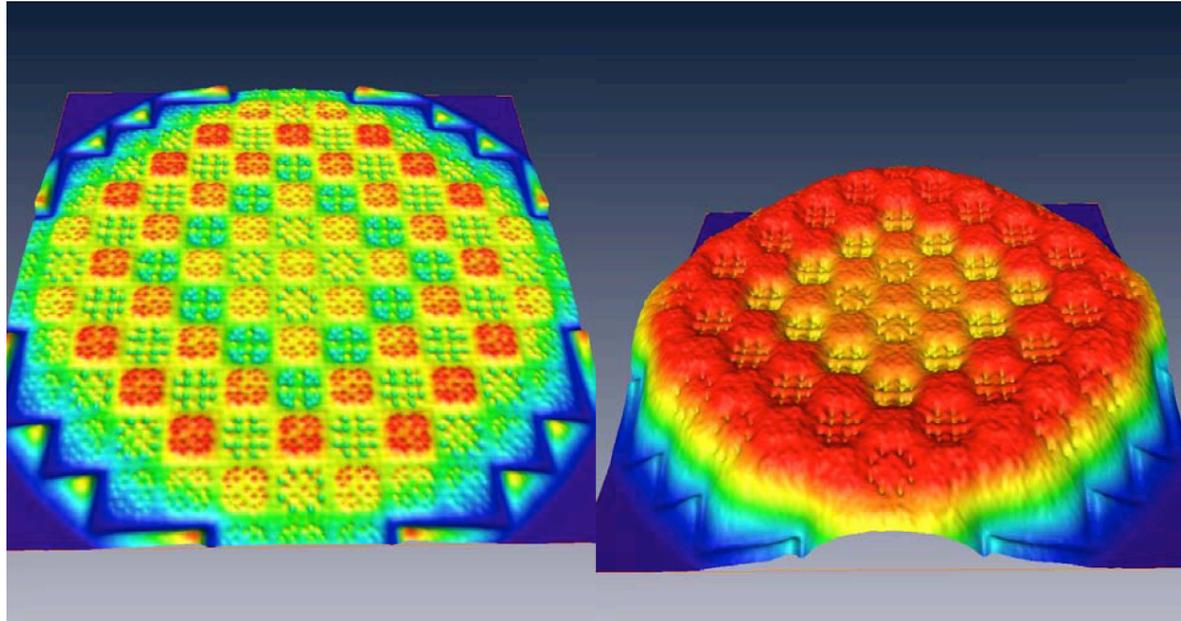


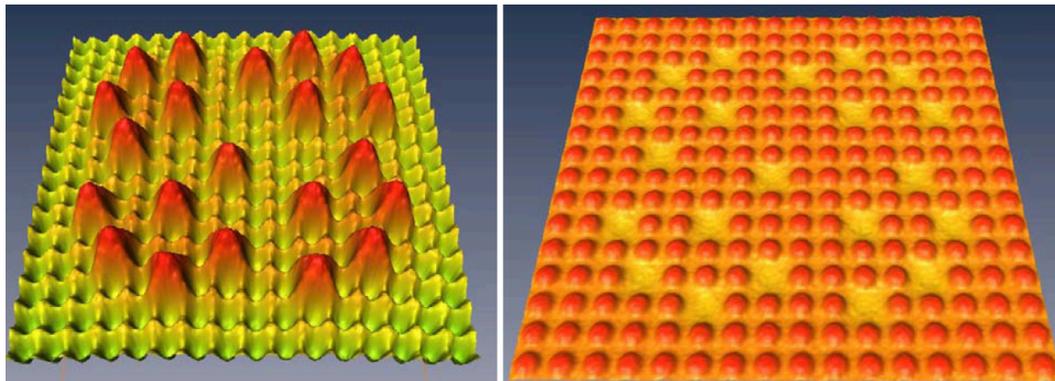
Figure 5. Incomplete HEU Sphere Reflected by Aluminum, heu-met-fast-012

MCNP & Reactors (1) - PWR Analysis

Whole-core Thermal & Total Flux from MCNP5 Analysis



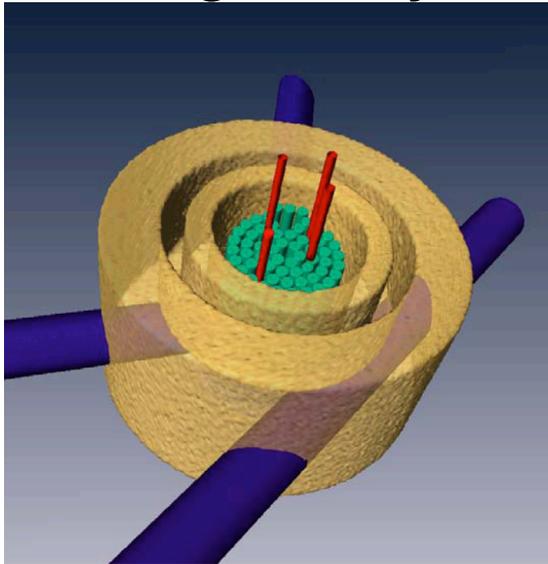
Assembly Thermal & Fast Flux from MCNP5 Analysis



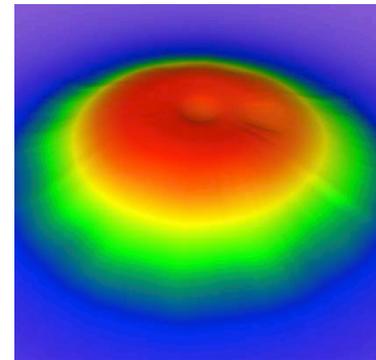
(from Luka Snoj, Jozef Stefan Inst.)

MCNP & Reactors (2) - TRIGA Reactor LEU Conversion

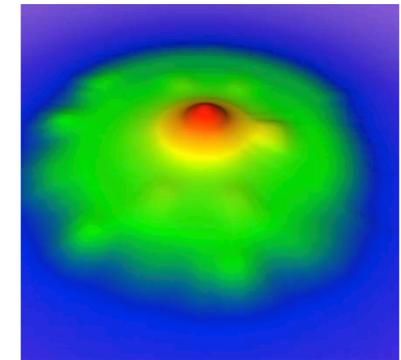
3D geometry



Fast Flux

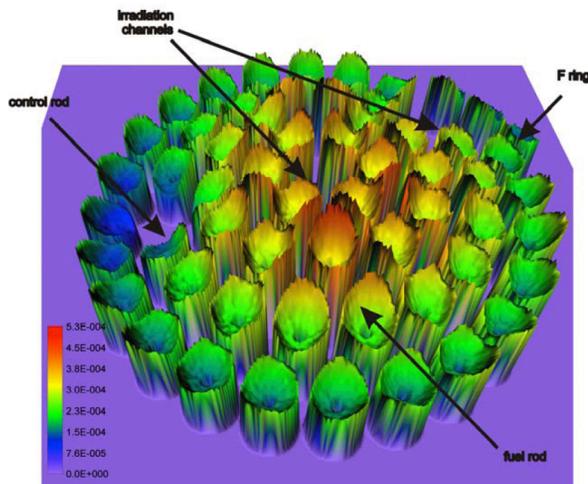
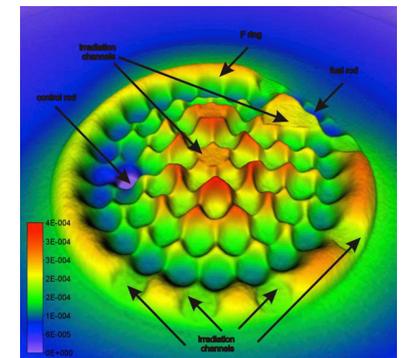
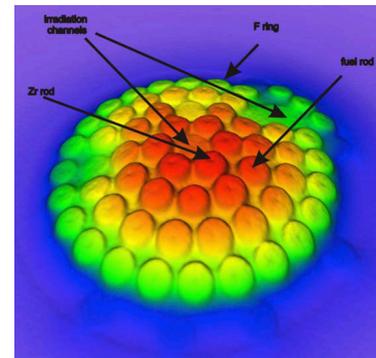


Thermal Flux



Diffusion
Theory
Codes

MCNP
Analysis



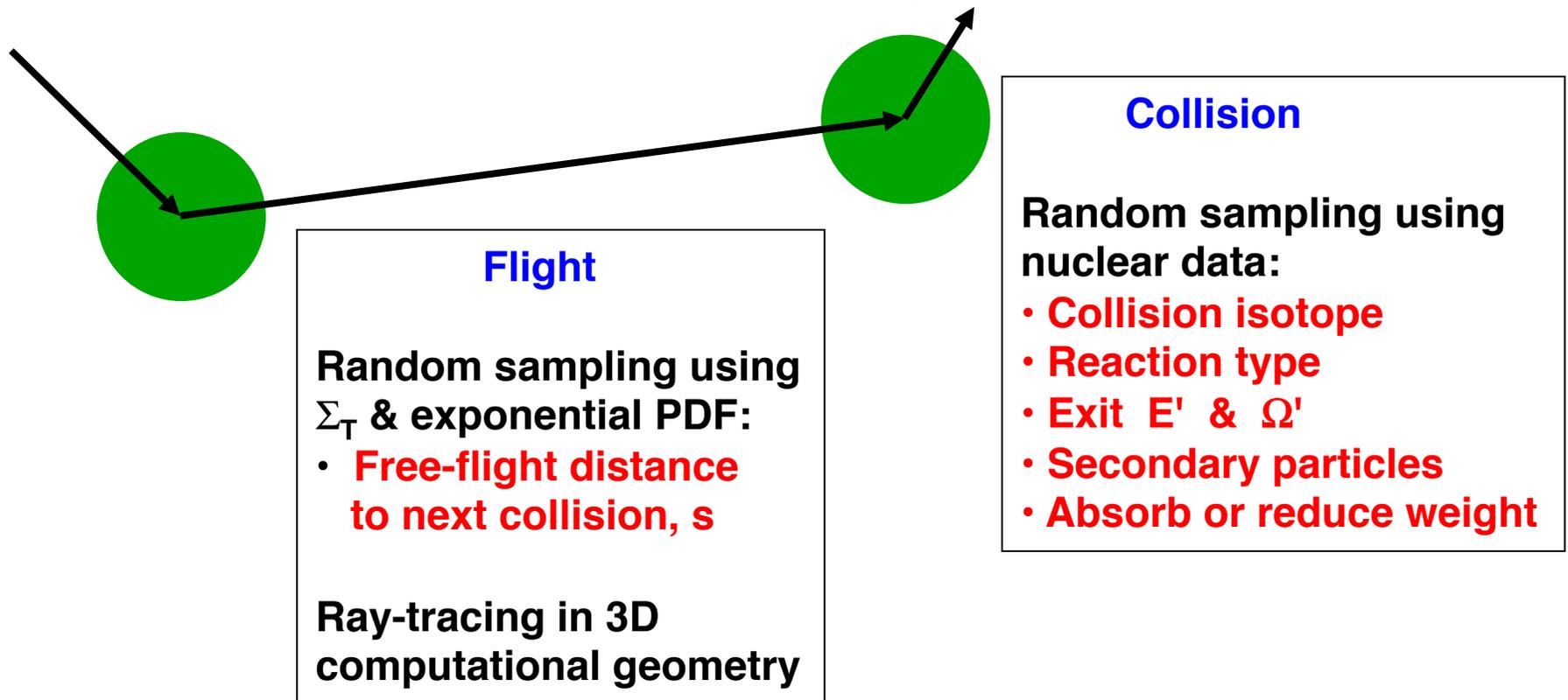
Radial Power Density
From MCNP Analysis

(from Luka Snoj, Jozef Stefan Inst.)

Monte Carlo Simulation & the Transport Equation

Monte Carlo - Introduction

- **Goal:** Simulate nature, particles moving through physical objects



During analysis of both flights & collisions, tally information about distances, collisions, etc. to use later in statistical analysis for results

Monte Carlo Calculations

- After a particle emerges from source or collision, or if the particle is entering a new cell:
 - Randomly sample **the free-flight distance** to the next interaction
 - If **distance-to-interaction < distance-to-boundary**, then move the particle to the interaction point
 - **Collision physics** at the interaction point:
 - Determine which **isotope** the interaction is with
 - Determine which **reaction type** for that isotope
 - Determine the **exit energy & direction** of the particle
 - Determine if **secondary particles** were produced
 - **Biasing** + weight adjustments
 - **Tallies** of quantities of interest

Sampling the Flight Distance

- Given a particle in a cell containing material M, sample the free-flight distance to the next interaction
 - Σ_T = total macroscopic cross-section in material M
= probability of any interaction per unit distance, units cm^{-1}

$$\Sigma_T(E) = \sum_k^{\text{nuclides in material}} N^k \cdot \sigma_T^k(E)$$

- PDF for flight distance s , where $0 \leq s \leq \infty$,

$$f(s) = \Sigma_T \exp(-\Sigma_T s)$$

- Sampling procedure

$$F(s) = 1 - \exp(-\Sigma_T s) \quad \rightarrow \quad s = -\ln(\xi) / \Sigma_T$$

Selecting the Collision Isotope

- $\Sigma_T = \sum_k N^k \sigma_T^k$ where $k =$ isotopes in material M

- **Probability that collision is with isotope J**

$$p_J = \frac{N^J \sigma_T^J}{\Sigma_T}$$

- $\{ p_J \}$ = set of discrete probabilities for selecting collision isotope

- $\{ P_J \}$ = discrete CDF, $P_J = \sum_{k=1}^J p_k$

- **Discrete sampling** for collision isotope k

table search to determine k such that $P_{k-1} \leq \xi < P_k$

Selecting the Reaction Type

- For collision isotope k ,

$$\sigma_T = \sigma_{\text{elastic}} + \sigma_{\text{inelastic}} + \sigma_{\text{capture}} + \sigma_{\text{fission}} + \dots$$

- $p_J = \sigma_J / \sigma_T =$ probability of **reaction type J** for isotope k
- $\{p_J\} =$ set of discrete probabilities for selecting reaction type **J**
- $\{P_J\} =$ discrete CDF,
$$P_J = \sum_{k=1}^J p_k$$
- **Discrete sampling** for reaction type **J**
table search to determine J such that $P_{J-1} \leq \xi < P_J$

Sampling Exit Energy & Direction

- **Given a collision isotope k & reaction type j , the random sampling techniques used to determine the exit energy and direction, E' and (u',v',w') , depend on**
 - Conservation of energy & momentum
 - Scattering laws - either equations or tabulated data
- **Examples**
 - Isotropic scattering in lab system
 - Elastic scattering, target-at-rest
 - Elastic scattering, free-gas model
 - Inelastic scattering
 - $S(\alpha,\beta)$ thermal scattering
 - Other collision physics, MCNP

Inelastic Scattering - MCNP

- Law 1 - ENDF law 1 - Equiprobable energy bins**
- Law 2 - Discrete photon energies**
- Law 3 - ENDF law 3 - Inelastic scatter from nuclear levels**
- Law 4 - ENDF law 4 - Tabular distribution**
- Law 5 - ENDF law 5 - General evaporation spectrum**
- Law 7 - ENDF law 7 - Simple Maxwell fission spectrum**
- Law 9 - ENDF law 9 - Evaporation spectrum**
- Law 11 - ENDF law 11 - Energy dependent Watt spectrum**
- Law 22 - UK law 2 - Tabular linear functions of incident energy out**
- Law 24 - UK law 6 - Equiprobable energy multipliers**
- Law 44 - ENDF law 1, lang 2, Kalbach-87 correlated energy-angle scatter**
- Law 61 - ENDF law 11, lang 0,12, or 14 - correlated energy-angle scatter**
- Law 66 - ENDF law 6 - N-body phase space distribution**
- Law 67 - ENDF law 7 - correlated energy-angle scatter**

Other Collision Physics - MCNP

- **Emission from fission**
- **Delayed neutron emission**
- **S(α,β) scattering for thermal neutrons**
- **Free-gas scattering for neutrons**
- **Probability tables for the unresolved resonance energy range**

- **Photon interactions**
 - Photoelectric effect
 - Pair production
 - Compton scattering (incoherent)
 - Thomson scattering (coherent)
 - Fluorescent emission
 - Photonuclear reactions

- **Electron interactions - condensed history approach**
 - Stopping power, straggling, angular deflections
 - Bremsstrahlung
 - K-shell impact ionization & Auger transitions
 - Knock-on electrons

Monte Carlo Simulation - Assumptions

Assume:

- Neutrons & photons are particles, not waves
- Particles move in a straight line between collisions (neutrons, photons)
- Collisions occur instantaneously, at a point in space
- Particle speeds are small enough to neglect relativistic effects
- Particle speeds are high enough to neglect quantum effects
- Particle collisions do not change the properties of a material (ie, no feedback, no material heating, no depletion)

Why?

- Want to solve the **linear** Boltzmann transport equation
- Want to apply the **superposition principle**
- Want the **Central Limit Theorem** to apply for computing statistics
 - Statisticians love the term “IID” - Independent, Identically Distributed

(Any or all of the above assumptions can be relaxed, with careful analysis & extra computing cost.)

Linear Boltzmann Transport Equation

- Time-dependent linear Boltzmann transport equation for neutrons, with prompt fission source & external source

$$\begin{aligned}
 \frac{1}{v} \frac{\partial \psi(\vec{r}, E, \vec{\Omega}, t)}{\partial t} = & \quad \text{External source} \quad Q(\vec{r}, E, \vec{\Omega}, t) + \quad \text{Scattering} \quad \iint \psi(\vec{r}, E', \vec{\Omega}', t) \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega} \cdot \vec{\Omega}') d\vec{\Omega}' dE' \\
 & + \quad \text{Multiplication} \quad \frac{\chi(\vec{r}, E)}{4\pi} \iint v \Sigma_f(\vec{r}, E') \psi(\vec{r}, E', \vec{\Omega}', t) d\vec{\Omega}' dE' \\
 & - \quad \text{Leakage} \quad \text{Collisions} \quad - \left[\vec{\Omega} \cdot \nabla + \Sigma_T(\vec{r}, E) \right] \cdot \psi(\vec{r}, E, \vec{\Omega}, t)
 \end{aligned}$$

$$\frac{1}{v} \frac{\partial \psi(\vec{r}, E, \vec{\Omega}, t)}{\partial t} = \underbrace{Q}_{\text{Gains}} + \underbrace{[S+M]}_{\text{Gains}} \cdot \psi - \underbrace{[L+T]}_{\text{Losses}} \cdot \psi$$

- This equation can be solved directly by Monte Carlo, assuming:
 - Each neutron history is an IID trial (independent, identically distributed)
 - All neutrons must see same probability densities in all of phase space
 - Usual method: geometry & materials fixed over solution interval Δt

- **Derive integral equation, in kernel form**

- **Start with integro-differential equation**

- **Use integrating factor** $\exp\left[-\int_0^R \Sigma_T(\vec{r} - R\hat{\Omega}, E) dR'\right]$, where $R\hat{\Omega} = \vec{r} - \vec{r}'$

- **Define**

$$\vec{E} = E \cdot \hat{\Omega}$$

Collision density: $\Psi(\vec{r}, \vec{E}) = \Sigma_T(\vec{r}, E) \cdot \psi(\vec{r}, \vec{E})$

Transport kernel: $T(\vec{r}' \rightarrow \vec{r}, \vec{E}) = \Sigma_T(\vec{r}, E) \cdot \exp\left[-\int_0^{|\vec{r}-\vec{r}'|} \Sigma_T(\vec{r}' + s\hat{\Omega}, E) ds\right] \cdot \frac{\delta(\hat{\Omega} \cdot \frac{\vec{r}-\vec{r}'}{|\vec{r}-\vec{r}'|} - 1)}{|\vec{r}-\vec{r}'|^2}$

Collision kernel: $C(\vec{E}' \rightarrow \vec{E}, \vec{r}) = \frac{\Sigma_S(\vec{r}, \vec{E}' \rightarrow \vec{E})}{\Sigma_T(\vec{r}, E')} + \frac{\chi(E) \nu \Sigma_F(\vec{r}, E')}{4\pi \cdot \Sigma_T(\vec{r}, E')}$

- **Then**

$$\Psi(\vec{r}, \vec{E}) = \int \left[\int \Psi(\vec{r}', \vec{E}') \cdot C(\vec{E}' \rightarrow \vec{E}, \vec{r}') d\vec{E}' + Q(\vec{r}', \vec{E}') \right] \cdot T(\vec{r}' \rightarrow \vec{r}, \vec{E}) d\vec{r}'$$

Basis for the Monte Carlo Solution Method

$$\Psi(\vec{r}, \vec{E}) = \int \left[\int \Psi(\vec{r}', \vec{E}') \cdot C(\vec{E}' \rightarrow \vec{E}, \vec{r}') d\vec{E}' + Q(\vec{r}', \vec{E}') \right] \cdot T(\vec{r}' \rightarrow \vec{r}, \vec{E}) d\vec{r}'$$

Let $p = (\vec{r}, \vec{E})$ and $R(p' \rightarrow p) = C(\vec{E}' \rightarrow \vec{E}, \vec{r}') \cdot T(\vec{r}' \rightarrow \vec{r}, \vec{E})$

Expand Ψ into components having 0,1,2,...,k collisions

$$\Psi(p) = \sum_{k=0}^{\infty} \Psi_k(p), \quad \text{with} \quad \Psi_0(p) = \int Q(\vec{r}', \vec{E}) \cdot T(\vec{r}' \rightarrow \vec{r}, \vec{E}) d\vec{r}'$$

By definition,

$$\Psi_k(p) = \int \Psi_{k-1}(p') \cdot R(p' \rightarrow p) dp'$$

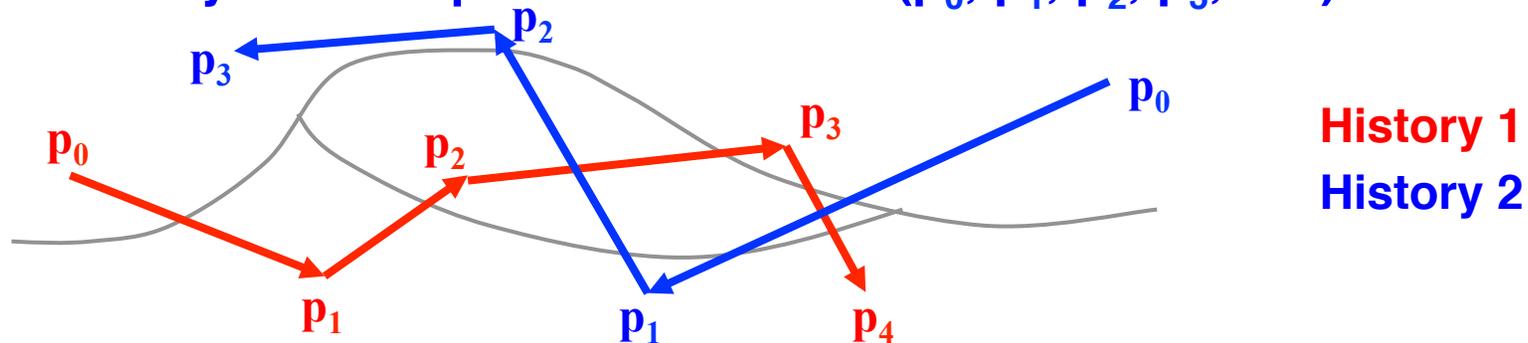
Markovian: collision k depends only on the results of collision $k-1$,
and not on any prior collisions $k-2, k-3, \dots$

Histories

- After repeated substitution for Ψ_k

$$\begin{aligned}\Psi_k(p) &= \int \Psi_{k-1}(p') \cdot R(p' \rightarrow p) dp' \\ &= \int \dots \int \Psi_0(p_0) \cdot R(p_0 \rightarrow p_1) \cdot R(p_1 \rightarrow p_2) \dots R(p_{k-1} \rightarrow p) dp_0 \dots dp_{k-1}\end{aligned}$$

- A "history" is a sequence of states $(p_0, p_1, p_2, p_3, \dots)$



- For estimates in a given region, tally the occurrences for each collision of each "history" within a region

$$\Psi_k(p) = \int \dots \int \Psi_0(p_0) \cdot R(p_0 \rightarrow p_1) \cdot R(p_1 \rightarrow p_2) \dots R(p_{k-1} \rightarrow p) dp_0 \dots dp_{k-1}$$

Monte Carlo approach:

- **Generate a sequence of states ($p_0, p_1, p_2, p_3, \dots$) [i.e., a history] by:**

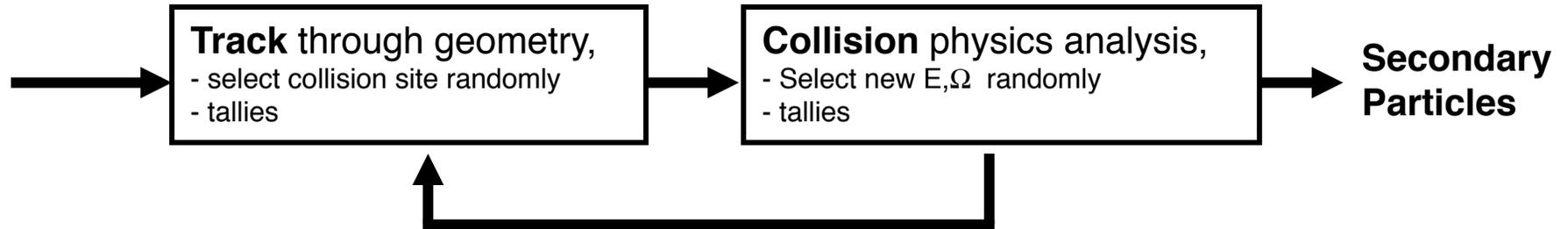
 - Randomly sample from PDF for source: $\Psi_0(p_0)$
 - Randomly sample from PDF for k^{th} transition: $R(p_{k-1} \rightarrow p_k)$

- **Generate estimates of results by averaging over states for M histories:**

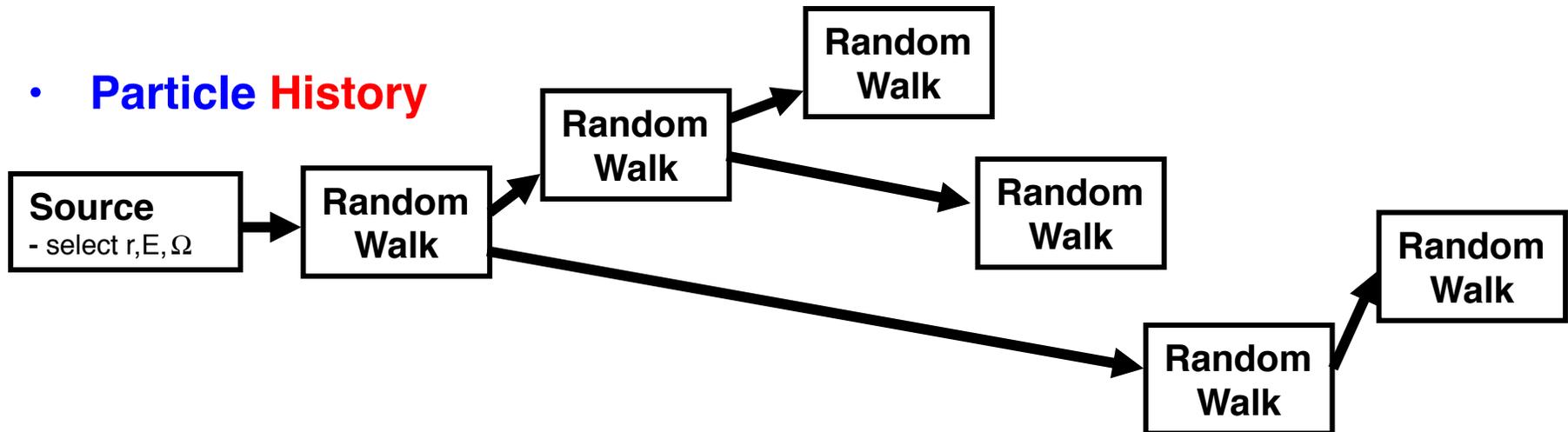
$$A = \int A(p) \cdot \Psi(p) dp \approx \frac{1}{M} \cdot \sum_{m=1}^M \left(\sum_{k=1}^{\infty} A(p_{k,m}) \right)$$

Particle Histories

- **Random Walk for Particle**

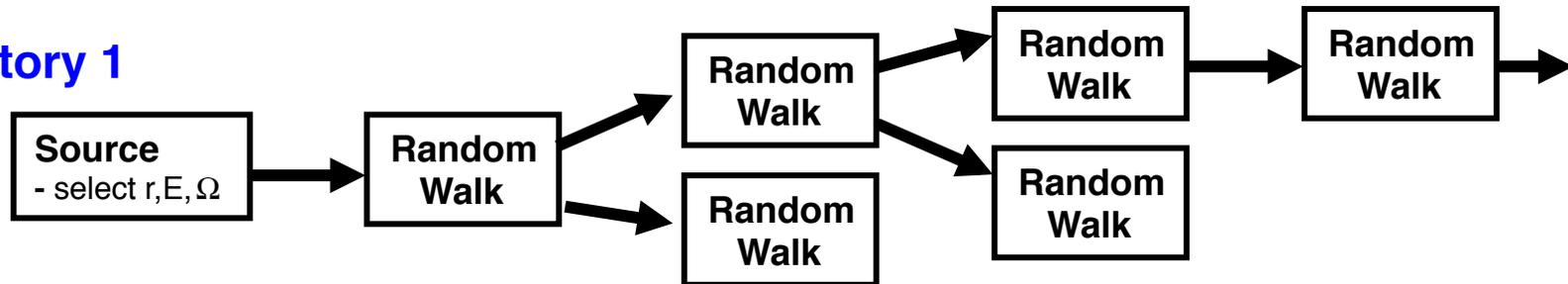


- **Particle History**

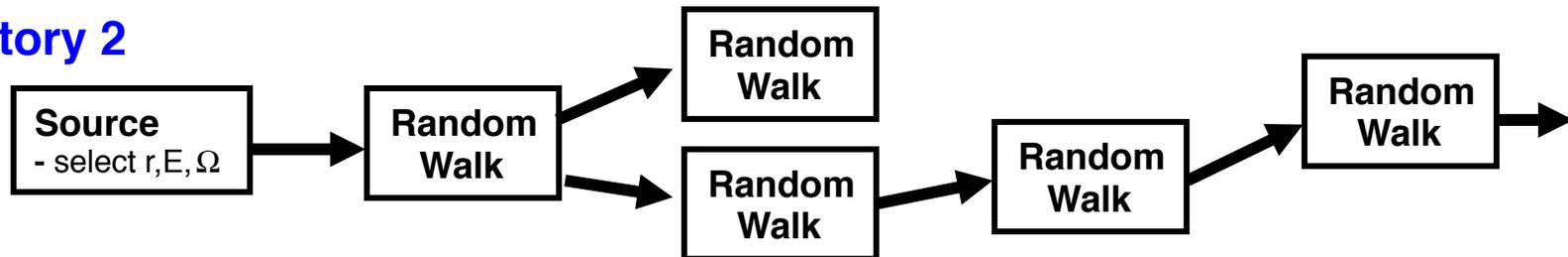


Fixed-source Monte Carlo Calculation

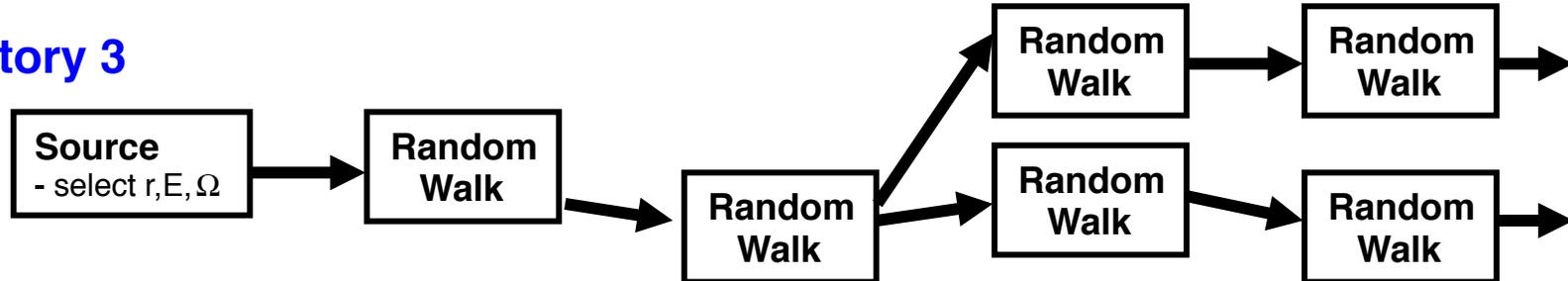
History 1



History 2



History 3



K_{eff} Eigenvalue Equation

- For problems with fission multiplication, another approach is to create a static eigenvalue problem from the time-dependent transport equation (the asymptotic or steady-state solution)
- Introduce K_{eff} , a scaling factor on the multiplication (ν)
- Assume:
 1. Fixed geometry & materials
 2. No external source: $Q(\mathbf{r}, E, \Omega, t) = 0$
 3. $\partial\Psi/\partial t = 0$: $\nu \Rightarrow \nu / K_{\text{eff}}$
- Setting $\partial\Psi/\partial t = 0$ and introducing the K_{eff} eigenvalue gives

$$[L + T] \Psi_k(\vec{r}, E, \vec{\Omega}) = \left[S + \frac{1}{K_{\text{eff}}} M \right] \Psi_k$$

- Steady-state equation, a static eigenvalue problem for K_{eff} and Ψ_k
- K_{eff} = effective multiplication factor
- K_{eff} and Ψ_k should never be used to model time-dependent problems.

K_{eff} Eigenvalue Equation

Leakage

Collisions

Scattering

$$\left[\vec{\Omega} \cdot \nabla + \Sigma_T(\vec{r}, E) \right] \cdot \psi(\vec{r}, E, \vec{\Omega}) = \iint \psi(\vec{r}, E', \vec{\Omega}') \Sigma_S(\vec{r}, E' \rightarrow E, \vec{\Omega} \cdot \vec{\Omega}') d\vec{\Omega}' dE'$$

Multiplication

$$+ \frac{1}{k_{\text{eff}}} \frac{\chi(E, \vec{r})}{4\pi} \iint v \Sigma_F(\vec{r}, E') \psi(\vec{r}, E', \vec{\Omega}') d\vec{\Omega}' dE'$$

$$[L + T] \Psi_k = [S + 1/k M] \Psi_k$$

- The factor $1/k$ changes the relative level of the fission source, to balance the equation & permit a steady-state solution

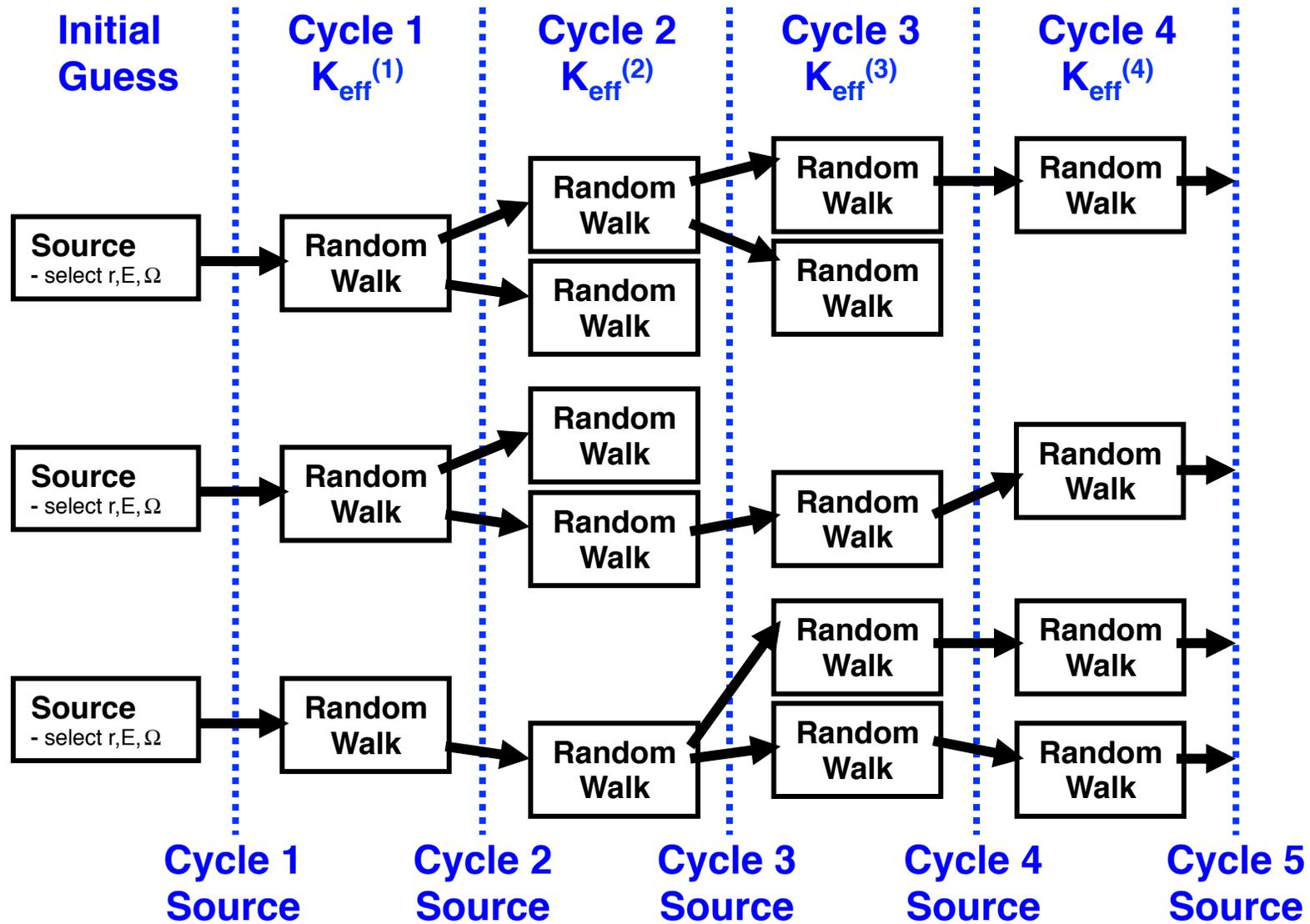
- **Criticality**

Supercritical: $K_{\text{eff}} > 1$

Critical: $K_{\text{eff}} = 1$

Subcritical: $K_{\text{eff}} < 1$

Monte Carlo Eigenvalue calculation



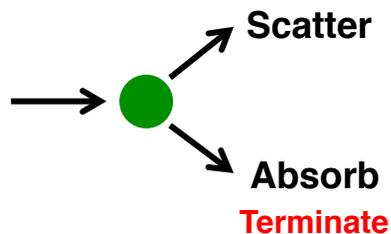
Iterate (cycle) until converged, then more to accumulate tallies

**Using
Expected-value Outcomes
VS
Detailed Modeling**

Analog vs Weighted Simulations

- **Monte Carlo methods evaluate integrals using random sampling**
 - Random sampling introduces variance (noise) into the results
 - More random sampling in the simulation → more variance
- **Statistical weights for particles can be used to permit replacing the random sampling of an event by the expected value for the event**

Analog Simulation



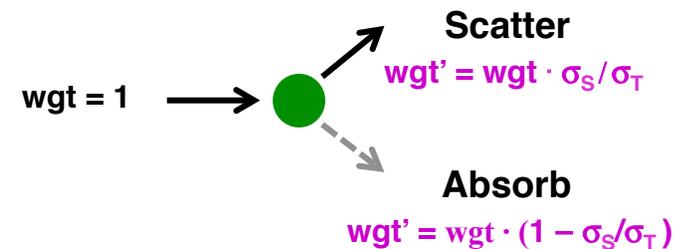
Random selection of scatter vs absorb.

Estimate absorption for N collisions:

```
S = 0
For k = 1 ... N {
    if  $\xi > \sigma_S / \sigma_T$  then S += 1
}
```

Absorption = S / N + statistical noise

Weighted Simulation



Always scatter, with reduced wgt.

Estimate absorption for N collisions:

$$\text{Absorption} = [N \cdot (1 - \sigma_S / \sigma_T)] / N = \sigma_S / \sigma_T$$

Replacing random sampling of an event by the expected value eliminates the variance contribution from the event.

Typical Examples of Weighted Simulation

- **Doppler broadening**
 - For neutron flights through a material, we don't randomly sample target nuclide velocity for the $\sim 10^{20}$ nuclides in the flight path
 - We average the target nuclide cross-sections over a Maxwellian distribution of nuclide velocities, and use the average cross-section to determine the flight distance
 - **Criticality safety & reactor physics**
 - We routinely use “implicit capture”, where neutrons always survive a collision with weight reduced by σ_S / σ_T
 - Some codes (not MCNP) model n-2n by scattering and multiply neutron weight by 2.
 - For neutrons produced by fission, routinely use expected value of $\text{wgt} \cdot v \Sigma_F / \Sigma_T$ neutrons per collision
 - For photon production, routinely use $\text{wgt} \cdot \sigma_{n \rightarrow \gamma} / \sigma_T$ photons produced per collision
- Use of expected values implies uncorrelated outcomes**

Selecting the Reaction Type - Modified

- In many applications, **survival biasing** is an effective variance reduction technique
 - Survival biasing is also called implicit absorption, nonabsorption weighting, or (loosely) implicit capture
 - $\Sigma_T = \Sigma_{\text{absorption}} + \Sigma_{\text{scatter}}$ (absorption = disappearance)
 - Probability that particle survives collision = $P_{\text{surv}} = \Sigma_{\text{scatter}} / \Sigma_T$
 - Probability that particle is absorbed (killed) = $1 - P_{\text{surv}}$
- Disallow absorption of particle, & then adjust particle weight to ensure a fair game
 - Tally absorption of $\text{wgt} \cdot (1 - P_{\text{surv}})$
 - Multiply particle weight by P_{surv}
 - When selecting collision isotope: **use Σ_S 's, not Σ_T 's for isotopes**
 - When selecting reaction type: **don't include σ_A**

Secondary Particle Creation

- Consider a collision which results in fission

$$\text{wgt} \cdot \nu \Sigma_F / \Sigma_T = \text{expected number of fission neutrons produced per collision}$$

- To sample the number of neutrons produced in the collision

- Let $r = \text{wgt} \cdot \nu \Sigma_F / \Sigma_T$
 $n = \text{int}[r]$

- Then, Produce n fission neutrons with probability 1 ,
and an additional fission neutron with probability $r-n$

- Example: $\text{wgt} \cdot \nu \Sigma_F / \Sigma_T = 1.75$

If $\xi < .75$, produce 2 neutrons, otherwise produce 1
or
Produce $\text{int}[1.75 + \xi]$ neutrons

Fission Process Modeling in MCNP6

- **Terrell**

- **probability for producing n fission neutrons**

$$P_0 = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{1/2} \exp\left(\frac{-(x - \bar{\nu} + b)^2}{2\sigma^2}\right) dx ,$$

$$P_{n \neq 0} = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{n-1/2}^{n+1/2} \exp\left(\frac{-(x - \bar{\nu} + b)^2}{2\sigma^2}\right) dx$$

- **Random sampling from a continuous Gaussian is easy**
- **Converting to integer is trivial, but does not preserve moments**
- **b = small adjustment, to preserve correct nu-bar**
- **Traditional MCNP6 options differ only in schemes for sampling a Gaussian, converting to integer, & adjusting to preserve nu-bar**

- **Measured data**

- **Terrell**
- **Zucker, Holden**
- **Gwin, Spencer, Ingle**

- **Lestone method based on preserving moments**

MCNP6 – KCODE Calculations

- **For criticality calculations** [no external source, no spontaneous fission]
 - Neutron multiplicity for fission is based on **expected value** of **$wgt \cdot \nu \Sigma_F^{mat} / \Sigma_T^{mat}$** neutrons per collision in the material
 - If more than 1 neutron, the energy & direction for each are sampled independently (no correlation)
 - The spectrum used for the fission neutrons is randomly chosen using probabilities **$\nu \Sigma_F^{iso} / \nu \Sigma_T^{mat}$** for the nuclides in the material
 - Energy is sampled using ENDF spectrum data for the selected nuclide
 - Prompt vs delayed neutron selected first, then energy
 - If more than 1 neutron, energy is sampled **independently** for each one (no correlation), using the same spectrum data
 - The direction for fission neutrons is sampled **isotropically**
 - If more than 1 neutron, directions are sampled **independently** for each neutron (no correlation in direction)
 - For KCODE problems with photons, photons are sampled **independent** of neutrons (no correlation between neutrons & photons)

- **Why is the expected value approach to fission neutron production used for criticality calculations? Why not use explicit fission neutron multiplicity data?**
 - Traditional MC work in the criticality safety community has focused on k-effective, reflector & control material reactivity, etc.
 - The reactor physics community has traditionally used MC for k-effective, power distributions, control material reactivity, etc.
 - Very extensive collections of verification-validation data, MC vs benchmark experiments for those applications
 - **No verification-validation work has been done to date on using explicit fission neutron multiplicity options in MCNP for criticality safety or reactor physics applications**

MCNP6 – Fixed-Source Calculations

- For fixed-source problems, MCNP6 has a variety of options for treating fission neutron **multiplicity**
- **FMULT** input card sets the option for each fissionable nuclide:
 - **Spontaneous fission:**
 - Multiplicity: nu-bar + Gaussian width **or** 10-bin distribution
 - Spectrum: Watt spectrum
 - **Induced fission:**
 - MCNP traditional, based on expected value, $\nu \Sigma_F^{\text{mat}} / \Sigma_T^{\text{mat}}$
 - Explicit multiplicity model options:
 - Method
 - » Lestone model (based on fits to moments)
 - » **Ensslin/Santi/Beddingfield/Mayo model**
 - » LLNL fission package (many options)
 - Data
 - » Terrell
 - » Lestone
 - » **Ensslin/Santi/Beddingfield/Mayo**
 - Shift
 - » Various options, preserves nu-bar
(needed when sampling integers from continuous distribution)

Spontaneous Fission – Default Data

fission multiplicity data.

zaid	width	watt1	watt2	yield	sfnu	CDF for number of neutrons														
90232	1.079	.800000	4.00000	6.00E-08	2.140															
92232	1.079	.892204	3.72278	1.30E+00	1.710															
92233	1.041	.854803	4.03210	8.60E-04	1.760															
92234	1.079	.771241	4.92449	5.02E-03	1.810															
92235	1.072	.774713	4.85231	2.99E-04	1.860															
92236	1.079	.735166	5.35746	5.49E-03	1.910															
92238	1.230	.648318	6.81057	1.36E-02	0.048	.297	.722	.950	.993	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
93237	1.079	.833438	4.24147	1.14E-04	2.050															
94236	0.000	.000000	0.00000	0.00E+00	0.080	.293	.670	.905	.980	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
94238	1.115	.847833	4.16933	2.59E+03	0.056	.267	.647	.869	.974	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
94239	1.140	.885247	3.80269	2.18E-02	2.160															
94240	1.109	.794930	4.68927	1.02E+03	0.063	.295	.628	.881	.980	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
94241	1.079	.842472	4.15150	5.00E-02	2.250															
94242	1.069	.819150	4.36668	1.72E+03	0.068	.297	.631	.879	.979	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
95241	1.079	.933020	3.46195	1.18E+00	3.220															
96242	1.053	.887353	3.89176	2.10E+07	0.021	.168	.495	.822	.959	.996	.999	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
96244	1.036	.902523	3.72033	1.08E+07	0.015	.131	.431	.764	.948	.991	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
96246	0.000	.000000	0.00000	0.00E+00	0.015	.091	.354	.699	.917	.993	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
96248	0.000	.000000	0.00000	0.00E+00	0.007	.066	.287	.638	.892	.982	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
97249	1.079	.891281	3.79405	1.00E+05	3.400															
98246	0.000	.000000	0.00000	0.00E+00	0.001	.114	.349	.623	.844	.970	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
98250	0.000	.000000	0.00000	0.00E+00	0.004	.040	.208	.502	.801	.946	.993	.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
98252	1.207	1.180000	1.03419	2.34E+12	0.002	.028	.153	.427	.733	.918	.984	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
98254	0.000	.000000	0.00000	0.00E+00	0.000	.019	.132	.396	.714	.908	.983	.998	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
100257	0.000	.000000	0.00000	0.00E+00	0.021	.073	.190	.390	.652	.853	.959	.993	1.00	1.00	1.00	1.00	1.00	1.00	1.00	
102252	0.000	.000000	0.00000	0.00E+00	0.057	.115	.207	.351	.534	.717	.863	.959	.997	1.00	1.00	1.00	1.00	1.00	1.00	

MCNP6 – Induced Fission Neutron Multiplicity Options

- Overly complicated – a result of recent merging of MCNP5 & MCNPX multiplicity treatments

Comments from the MCNP6 routine acenus.F90:

```
! Integer variable ifisnu determines the fission multiplicity
! dataset for sampling the Gaussian width.
!   ifisnu = abc
!     c = 1  Lestone data
!     c = 2  Terrell data
!     c = 3  Ensslin, Santi, Beddingfield, Mayo data
!     b = 0  MCNP5 shift to preserve nubar
!     b = 1  MCNPX shift to preserve nubar
!     b = 2  MCNPX threshold shift to preserve nubar
!     b = 3  MCNPX no shift to preserve nubar
!     b = 4  MCNPX nearest integer but with multiplicity prints
!     a = 0  MCNP5 normal_dist_sc Gaussian sampling
!     a >= 1 MCNPX normal_dist_po Gaussian sampling
!     a >= 2 MCNPX nu = nu + rang(), not MCNP5 nu = nu + half
```

- Similar options & more also from LLNL Fission package in MCNP6

- **LLNL fission model**
 - Fission neutrons & photons are correlated & have multiplicities
 - Includes all multiplicity measurements from literature. Empirical models used if data are not available
 - Neutrons and gammas sampled independently, no correlation
 - Scales multiplicity data to match $\bar{\nu}$ from evaluated data libraries
 - Neutrons & gammas emitted isotropically
- **Neutron induced fission data**
 - **4 options for neutron multiplicity**
 - Fit to Zucker-Holden data, 5th order polynomials in E_n
 - Same + Gwin-Spencer-Ingle data for ^{235}U at thermal energies
 - Valentine polynomial fit of $P_\nu(\bar{\nu})$, Zucker-Holden & Gwin-Spencer-Ingle
 - Tables from Zucker-Holden & Gwin-Spencer-Ingle data, statistical selection to nearest nu-bar, or Terrell if nu-bar out of range
 - **Spectrum**
 - Watt spectrum, TART scheme [b=1, fit a to poly in E_{in}]
 - **Neutron energy conservation, 3 options**
 - Independent, no energy conservation
 - Sample total neutron energy from Gaussian, rescale each neutron E
 - Sample total neutron energy from quadratic fit, rescale each neutron E

Example — Watt Spectrum

$$f(x) = \frac{2e^{-ab/4}}{\sqrt{\pi a^3 b}} e^{-x/a} \sinh \sqrt{bx}, \quad 0 < x$$

Rejection (*mcnp*)

- Based on Algorithm **R12** from 3rd Monte Carlo Sampler, Everett & Cashwell
- Define $K = 1 + ab/8$, $L = a \{K + (K^2 - 1)_{1/2}\}$, $M = L/a - 1$
- Set $x \leftarrow -\log \xi_1$, $y \leftarrow -\log \xi_2$
- If $\{y - M(x + 1)\}^2 \leq bLx$, accept: return (Lx)
otherwise, reject

Direct (*new vim*)

- Sample from Maxwellian in C-of-M, transform to lab

$$w \leftarrow a \left(-\log \xi_1 - \log \xi_2 \cos^2 \frac{\pi \xi_3}{2} \right)$$

$$x \leftarrow w + \frac{a^2 b}{4} + (2\xi_4 - 1) \sqrt{a^2 b w}$$

(assume isotropic emission from fission fragment moving with constant velocity in C-of-M)

- Unpublished sampling scheme, based on original Watt spectrum derivation

Not widely known –
not used in MCNP

MCNP6 – Work in Progress

- **For many years, patches to MCNP have existed for**
 - **Coincidence counting of fission neutrons**
 - Plan to incorporate the patches permanently into public version
 - **Intrinsic sources – spontaneous fission**
 - Plan to incorporate the patches permanently into public version
 - **List-mode data**
 - Can make use of exactly the same post-processing methods as for experimental data
- **CGMF package will be added to MCNP6**
- **Investigate use of multiplicity for MCNP criticality calculations (KCODE)**

References

Monte Carlo References

700+ technical reports, presentations, etc., are available from the MCNP website – mcnp.lanl.gov, under “Reference Collection”

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